T=0 Neutron-Proton Correlations at high angular momenta[1]

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Abstract. The properties of $T=0$ neutron-proton correlations are discussed within the framework of different model calculations. Single-j shell calculations reveal that the $T=0$ correlations remain up to the highest frequencies. They are more complex than the $T=1$ corrlations and cannot be restricted to $L=0$ pairs only. Whereas it may be difficult to find clear evidence for $T=0$ pairing at low spins, $T=0$ correlations are found to induce a new excitation scheme at high angular momenta.

INTRODUCTION

Pairing correlations have always played a decisive role for the low energy structure of atomic nuclei. In close analogy to the BCS-theory of superconductivity, it was suggested early on that the ground state of most nuclei is formed by a coherent superposition of pairs of nucleons, moving in time reversed orbits. [1] Although the BCS-theory of the nuclear pairing interaction is charge independent, one in general considers only scattering between pairs of like particles (neutron-neutron and proton-proton).

Atomic nuclei are composed of two different kind of fermions which can occupy identical states. This is an unique situation, that is not found in other fermionic systems. Since the short range nuclear force is attractive, nuclei in close vicinity of the $N = Z$ line may form a condensate of neutron-proton (np) pairs that have totally symmetric wave-functions in spin and ordinary space. Different approaches to generalize the pairing interaction to fully take into account the iso-spin degree of freedom have been discussed in the literature in the 60ties and 70ties, see e.g. Ref. [2] and references therein. Following the experimental observation of ^{100}Sn and the spectroscopic study of a large number of heavy $N = Z$ nuclei in recent years, the quest for neutron-proton pairing has gained renewed interest. [3–5] Indeed, the massdefect at the $N = Z$-line, the so called Wigner energy finds a microscopic explanation in a generalized pairing theory [4]. In the following we use the standard notations for isospin (t, T), intrinsic spin (s, S), orbital angular momentum (l, L) and total angular momentum (j, J), where small letters denote the single particle content and capital letters the vector added quantities.

Pairs of particles moving in time-reversed orbits have the largest momentum exchange when their total spin S and angular momentum L are coupled to zero. Such pairs form a triplet in iso-space $T = 1$, being decomposed of either proton (neutron-) pairs with $T_z = \pm 1$ or a neutron-proton pair with $T_z = 0$. Strong short range correlations of particle-particle (pp) type, are in general treated by means of the standard 'monopole' pairing force $(T=1)$ with $T_z = \pm 1$ pairs only. In order to treat protons and neutrons on the same footing, one may extend the formalism to include $T_z = 0$ pairs. [6] For even-even nuclei, such extensions may be considered less interesting, since the $T_z = 0$ pairs are simply related to $T_z = \pm 1$ pairs via rotation in iso-space. The binding energy of even-even nuclei e.g. is not affected by the inclusion of $T_z = 0$ pairing [4]. However, for odd-odd $N = Z$ nuclei, many interesting properties may emerge, that will be addressed in a forthcoming paper [7].

In nuclear physics it is well known that the Deuteron is bound only in the spin triplet, $S=1$ iso-spin singlet, $T=0$ state. Also nucleon-nucleon scattering data show stronger attraction for the spin triplet than spin singlet state. One may therefore expect that neutron-proton pairing is more important at the $N = Z$ line than neutron-neutron and proton-proton pairing.

In the context of the shell model, one defines a 'monopole' pairing interaction for the $L = 0$, $T = 1$ singlet state [8], and one may proceed in an analoguous manner for the $T = 0$, $L = 0$ and $S = 1$ triplet state. This restricted definition is of advantage for algebraic models [9–11] since it limits the model-space when analyzing properties of

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FIGURE 1. Decomposed (J, T) pairing energy for 2 protons and 2 neutrons in the $f_{7/2}$ shell. The results for 4 protons and 4 neutrons is similar.

np-correlations. It may be appealing, to consider $L=0$ pairs only for the pairing interaction. However, this neglects several important aspects. Whereas the $L=0$ part of a short range $T=1$ interaction like the δ-force is dominant, it plays only a minor role for the $T=0$ interaction [8]. This is nicely seen in the experimental spectra of odd-odd nuclei, where the low-lying 0^+-state is in close vicinity to states with odd spins and even parity corresponding to the $(j^2)_{J=1}$ and $(j^2)_{J=2j}$ configuration.

For mean field calculations, it does not make much sense to restrict to a $L=0$ pairing force, especially not for the $T=0$ channel. Already the $T=0$ pair with lowest J, $J=1$ has a strong $L=2$ component that needs to be taken into account. Not even the $T=1$ pairing channel can be restricted to $L=0$-pairing, when one aims at a quantitative description of the rotational motion and pair-breaking mechanism in deformed nuclei. One has to include at least $L=2$ ('quadrupole'-)pairing [14,15]. The contribution to the binding energy steming from the $L=2$-pairing may be negligible small, of the order of a tens of keV, but it is certainly coherent [15].

In the present paper, we investigate the influence of the $T=0$ correlations on properties of rotational bands at high angular momenta. Single-j shell calculations are presented in section 1 and mean-field calculations based on the HFB-method in section 2.

NEUTRON-PROTON CORRELATIONS IN A SINGLE-J SHELL

In a single-j shell, one can diagonalize exactly the two-body interaction and also investigate the dependence of different correlations on angular frequency [16]. The pair-gap, is not defined in such a model. Nevertheless, one may decompose the expectation value of the two-body interaction, E_{exp}, with respect to the contributions coming from the different angular momenta J. We have performed a single-j shell calculation for different number of particles in the $f_{7/2}$ shell and relate a 'gap'-parameter Δ_{JT} to the expectation energy via the following equation

$$E_{exp} = \frac{1}{2} \sum_{JT} \frac{\Delta_{JT}\Delta_{JT}^*}{E_{JT}}, \tag{1}$$

where E_{JT} is the value of the normalized, anti-symmetric two-body matrix elements of the δ-function interaction [17]. As expected, the single-j shell calculations indeed result in a strong binding for maximum and minimum J in the $T=0$ channel, but also shows that states with intermediate J are important, see fig. 1. Whereas the binding for the $T=0$-pairs is rather complex, the $T=1$ part of the interaction is dominated by a single J. It is the dominant role of the $J=0$ pairing in the $T=1$ channel that may justify the restriction to $L=0$ in that channel. These

properties of the $T=1$ and $T=0$ correlations have been known since long [8,18], see also the recent investigation in [19]. When we start to rotate the nucleus, the Coriolis force tends to align the quasi-particles along the rotational axis, resulting in the well known pair breaking mechanism. The $T=1$ pairing becomes reduced and the $L=0$ part totally quenched. Since the $J=1$ part of the $T=0$ correlations also involve particles in which the intrinsic j's are mainly coupled antiparallel, this part is reduced in a similar fashion as the $J=0$ correlations. At the same time, the $J=7$ correlation pick up in strength and compensate the loss from the $J=1$. Although there exist only one $J=7$ state in the $f_{7/2}$ shell, this state has the highest degeneracy, $2J+1$, implying that many pairs may contribute coherently to this state. The total $T=0$ correlations remain unchanged as a function of frequency. Apparently, the $T=0$ energy is not affected by rotation and indeed, we do not observe any effect on the alignment by switching on or off that part of the interaction.

Recent shell model calculations question the importance of $T=0$ correlations for the spectrum of ^{48}Cr [12]. However, the only matrix elements considered in this analysis are those of $L=0$. As shown above, in contrast to the $T=1$ channel, the $T=0$ interaction is most attractive for parallel $J=2j$ and antiparallel $J=1$ coupling of the individual angular momenta j, Fig. 1. Even the $T=0$, $J=1$ matrix element contains contribution from both $L=2$ and $L=0$. The requirement of total $L=0$ and $S=1$ for a l^2-pair of $T=0$ implies that the individual projection of the orbital angular momentum, l, (l_m) have to be antiparallel and the individual spins parallel. For a given l^2 configuration, one may couple the individual orbital angular momenta and intrinsic spins s, to a total angular momentum j, $j=l\pm 1/2$. When decomposing the contribution to the $L=0$ multiplet in terms the 'spin-orbit' partner pairs $(j=l+\frac{1}{2},\ j=l-\frac{1}{2})$, pairs with $(j=l+1/2)^2$ and $(j=l-1/2)^2$, respectively, we find from the appropriate $6j$ symbols a ratio of $8{:}7{:}2$ (for $l=2$). This implies of course, that the $L=0$, $T=0$ pairing becomes strongly reduced by the nuclear mean-field in the presence of the spin-orbit interaction. The concept of a restricted $L=0$, $T=0$ pairing may be meaningful up to the sd-shell, where the LS-coupling still has validity. When entering the $f_{7/2}$ shell, we do not expect the $L=0$-pairing in the $T=0$ channel to play a very important role. Therefore, it is not at all surprising that this interaction turns out to have little influence on the spectrum of ^{48}Cr.

One should remember, that the definition of the pairing gap originates from the mean-field approximation where it defines the average gap or potential felt by a pair of particles at the Fermi-surface [1,20,21]. The pairing interaction is thus intimately linked to the symmetry-breaking of the mean-field approach, which strictly separates between a particle-particle (pp) and particle-hole (ph) field. In contrast, the two-body 'pairing' matrix element of the shell-model is a different entity containing both particle-hole and particle-particle part and one has to be carefule when comparing results of the two different approaches. The question of a static pair-gap in the $T=0$ channel can be addressed meaningfully in the mean-field: if the correlations are strong enough, it will show up in a 'deformed' solution, otherwise not. This is of course linked to the strength of the interaction, which still needs to be determined. Generalized BCS- and HFB- calculations clearly indicate that $T=0$ correlations are coherent and necessary to understand the experimental data [2,4,13].

We are thus lead to the following conclusions: i)the spin-orbit force in the nuclear potential quenches part of the $L=0$ coupling and ii) the restriction to $L=0$ pairs only takes into account a minor fraction of the real correlations. To proper investigate the full spectrum of $T=0$, np-correlations, one needs to take into account all J-values (implying all possible L). The $T=0$ pairing as we define in the following, will have contributions from all J's. In an even-even nucleus e.g. the spin $I=0^+$ state has a contribution from the standard monopole-pairing with pairs of $J=0$ but of course also the contribution from all odd $J-$values. Note, however, that even the δ-force strongly simplifies the nucleon short-range interaction, since it allows only the coupling of even L's to take part. The interaction related to space antisymmetric states is not taken into account in any model involving a δ-force like interaction.

BAND TERMINATION AT HIGH ANGULAR MOMENTA

As discussed in the previous section, one may not see obvious fingerprints of the $T=0$ pairing in the low spin regime, since it is dominated by the breaking of pairs with low J and with respect to that, there is little difference in $J=0$ and $J=1$. In order to investigate the importance of the $T=0$ correlations at high angular momenta, we have performed a case study for the nucleus ^{48}Cr [13], that has been investigated quite extensively in experiment and theory [22,23]. The valence particles of ^{48}Cr are placed in the middle of the $f_{7/2}$ shell and the evolution of collective motion and band termination is well described by shell-model calculations [24]. The shell model faces difficulties to address states beyond the fp-shell. Hence, mean-field calculations may shed some light on the properties of states beyond the aligned $16\hbar^+$ state.

We have performed cranked HFB-calculations in R-space based on the Skyrme-force [25,26] where the two-body pp interaction has been extended to incorporate both the $T=0$ and $T=1$ channel [13]. The only symmetry restriction used in the calculations is parity [13]. In the low spin regime, we found two HFB-solutions, dominated by either the $T=0$ or $T=1$ correlations, that were almost degenerate in energy, see a) and b) in Fig.2. Note, that for the case

FIGURE 2. Comparison of calculated and experimentally deduced I_x as a funciton of rotational frequency, $\hbar\omega$. In a) we show two sets of calculations, with $G_{T0} = 1.1 G_{T1}$ and $1.3\ G_{T1}$. The low spin part, $I \leq 16\hbar$ has only $T = 1$ pairing, wheras above that spin value, a transition to $T = 0$ pairing occurs. In b) the HFB-solution is dominated by $T = 0$ pairing correlations, although a small part of $T = 1$ pairing is present simultanously. c) The contribution of the $T = 0$ pairing energy is added to the solution of a), according to $d\omega = \frac{dE_{pair}}{dI}$.

of the $T = 0$ solution, both pairing modes are present, showing the capability of our approach to incorporate the two different pairing channels simultanously. As shown in the previous section, the exact solution will always mix both pairing modes whereas the HFB approximation usually gives preference to either one. As discussed in ref. [4], particle number projection results in mixed solutions and one may expect that also iso-spin projection will become necessary. These steps will be considered in a further development of our model.

The results from the low-spin solutions appear very interesting: As seen in Fig. 2, the gross features of the alignment of the solution that is dominated by $T = 0$ pairing (b) does not differ very much from the solution with $T = 1$ (a). This underlines the previous discussion - the low spin regime will always be characterized by the pair-breaking mechanism - be it $J = 1$ or $J = 0$ pairs. Nevertheless, the slope of I_x at low spins of the $T = 0$ solution somewhat better reproduces the experimental values.

The small value of the moments of inertia of atomic nuclei have been taken as a fingerprint for the $T = 1$ pairing correlations, where the size of the reduction with respect to the value of the rigid body indicates the strength of the correlations. Apparently, in the low spin regime, we obtain a similar reduction for the $T = 0$-pairing, where again the size of the reduction is a measure of the correlations. Unfortunately, one cannot disentagle what is the contribution due to $T = 0$ and $T = 1$ pairing. Since the two solution are exptected to mix, we may artificially add the contribution of the pairing energy from the $T = 0$-pairing to the $T = 1$-solution. The result of such a mixing is shown in Fig. 2 c), resulting in a much improved agreement with experiment. To really investigate the effect of $T = 0$ and $T = 1$ pairing at low spins, one needs to go beyond the mean-field description.

In fig.3 the values of the pairing energy for the two solutions are compared. Indeed, the $T = 0$ pairing is considerably

more resistant to rotation than the $T=1$. The $T=0$ pairing energy reveal a similar drop as the $T=1$, but it does not approach zero and it increases again at the $12\hbar$ aligned state, which has a shape close to spherical. This dip in the pairing energy is related to the calculated backbend. Also the intrinsic quadrupole moments of the two solutions differ. For transitional nuclei, the difference can become quite large. The nucleus ^{44}Ti e.g. is calculated to have spherical shape in the presence of $T=1$ pairing whereas it has a calculated quadrupole moment of ≈ 50eb for the $T=0$ solution.
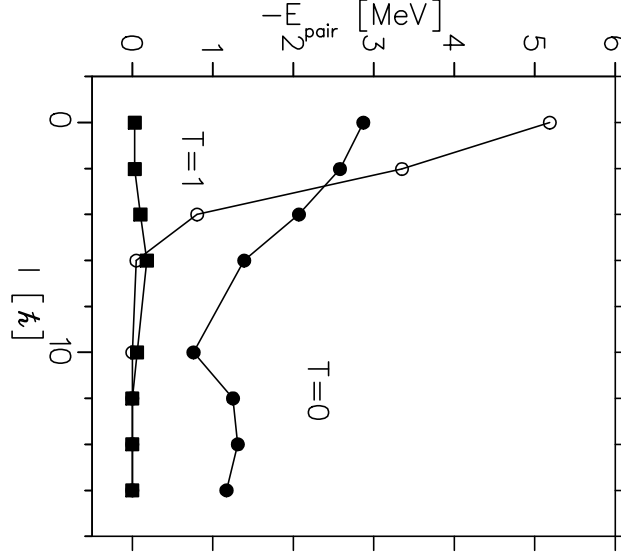
FIGURE 3. The pairing energy of the $T=0$ (solid symbols) and $T=1$ (open symbols) Skyrme-HFB solutions at low spins. Note the small value of the $T=1$ pairing for the $T=0$ solution.

The latter point is rather important and we will discuss it shortly. The pair-breaking mechanism is similar for $T=0$ and $T=1$, and one may not expect strong influence on the band-crossing frequencies. Nevertheless, since the $T=0$ pairing field affects the shape of the nucleus, and band-crossing frequencies quite sensitively depend on deformation [27], the two effects are linked together. For the case of ^{72}Kr e.g., a large delay of the band crossing has been observed [28]. A possible mechanism emerging from our result would be that the nucleus stays at a more deformed shape, thus delaying the crossing frequency. In addition, since in real nuclei more states than a single j-shell contributes to the pairing energy, one expects more binding from all different $J=1$ states, resulting in additional ground-state correlations.

For the high spin regime, we find only a solution with finite $T=0$ gap. This result clearly demonstrates the onset of $T=0$ pairing at high angular momenta, since the static $T=1$ correlations are quenched at these spin-values. The $T=0$ pairing energy rises after the terminating $I=16\hbar$-state and maximizes at $I=24\hbar$, where it has approximatively the same value as the nn (pp) $T=1$ pairing at $I=0\hbar$ (2.2 MeV). The size of the $T=0$ correlation implies the presence of a static $T=0$ pairing field. The increase in angular momenta beyond the terminating $I=16\hbar$ state is due to excitation from $d_{3/2}$ and $f_{7/2}$ into $g_{9/2}$ and $f_{5/2}$ orbits. Note that these particle-hole excitations are caused by the short range $T=0$ pairing force. Without the $T=0$ correlations, no cranked HFB- or HF-solutions are found in the region between $I=16$ and $I=32\hbar$ [13].

The   effect of the $T=0$ pairing is to allow for a smooth occupation of the aligned $[(d_{3/2})^{-2}_{3^+}(f_{7/2})^{-2}_{+1} - (f_{5/2})^2_{+5}(g_{9/2})^2_{9^+}]_{18^+}$ configuration (the $(f_{7/2})^{-2}$ holes are with respect to the $(f_{7/2})^8_{16^+}$ configuration). The occupation probability of this configurations is increasing smoothly, resulting in an almost constant increase in angular momenta and deformation as a function of frequency. Since the configuration is exactly half filled at $I=24\hbar$, we obtain a maximum for the pairing correlations at that spin value [13].

Note that this 'vertical' excitation is completely different to the common ph-excitations, that are associated with the shape coexisting band structures. One may e.g. promote 2 particles from the $d_{3/2}$ into the $g_{9/2}$. This 2p-2h excitation couples to angular momentum $I=0\hbar$ and may result in a new rotational band. In this case, the $g_{9/2}$
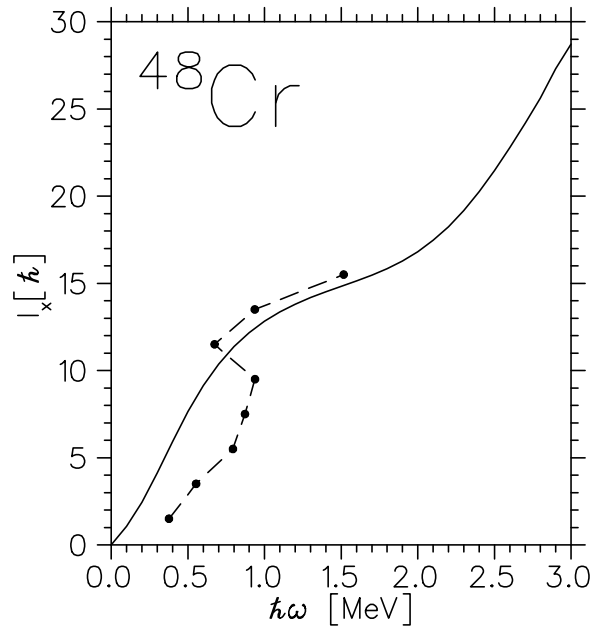
FIGURE 4. Cranked Woods-Saxon calculations for ^{48}Cr. The calculations are done at spherical shape and allow for both $T=0$ and $T=1$ pairing. The $T=0$ pairing field allows for a smooth occupation of the aligned deformation driving intruder orbitals

is fully occupied and the $d_{3/2}$ is empty and the angular momentum gain arises from the alignment of the valence particles. This kind of 'horizontal' ph-excitation form the well-know intruder bands or highly- and super-deformed band structures. In the case of the $T=0$ pairing, one instead smoothly occupies the aligned configuration, resulting in a smooth deformation change. This presents a new kind of collective excitations, where the $T=0$ pairing field induce an increase in deformation and angular momenta.

The same effect is seen in cranked Woods-Saxon calculations [7]. Here $T=0$ and $T=1$ pairing are present simultanously and contribute to the total energy. Approximate particle number projection is performed by means of the Lipkin Nogami procedure. More details can be found in [4,7]. An important difference of the cranked Woods-Saxon calculations is the lack of feed back from the ocupation of intruder orbitals to the single particle potential. Although the same configurations are occupied as in the cranked Skyrme-HFB calculations, the shape stays spherical, since the single particle potential does not feel the intrinsic deformation of the ph-excitations. Remarkably, the presence of $T=0$ pairing allows for a smooth increase of the angular momenta at spherical shape. Since we are cranking around a symmetry axis, this is in contrast to the step wise increase which is obtained for normal cranking with or without $T=1$, where each step in angular momentum is associated to the $<j_z>$ expectation value of each particular pair. The presence of $T=0$ pairing allows instead a smooth 'filling' of the aligned orbital. Again, we encounter a new mechanism to create angular momentum and deformation.

The feature discussed in this context is a general property of nuclei in the close vicinity of $N=Z$. Cranked HFB calculations for ^{44}Ti e.g. show the same mechanism. After the terminating state at $I=12\hbar$, $T=0$ correlations start to show up, resulting in a further increase of the angular momenta. For the case of ^{44}Ti, the $T=0$-solution is considerably more deformed than the spherical $T=1$-solution. Again, we expect only one solution to be physical, but in the presence of $T=0$ correlations, there is a clear tendency to more deformed shapes, that shows up especially in transitional nuclei. In general, there will always be the mechanism to go beyond the terminating state by means of $T=0$ induced ph excitations. These 'vertical' excitations will of course have to compete with the 'horizontal' excitations, where by deforming the nucleus a particular set of favoured ph-excitations can lead to a more deformed shape and result in a new collective rotational band.

An interesting situation may arise at super-deformed shape in $N=Z$ nuclei. Cranked Woods-Saxon calculations predict very deep minima at super- and hyperdeformed shapes in ^{88}Ru and ^{92}Pd. The very stable shapes of these doubly magic super- and hyper-deformed nuclei have similar configuration as the harmonic oscillator at 2:1 shape for $N=Z=40$. The experimental investigation of this shell structure is still in progress, but we may expect with the event of radio-active beam facilities to probe such exotic nuclei. Since the valence shell is particular large for
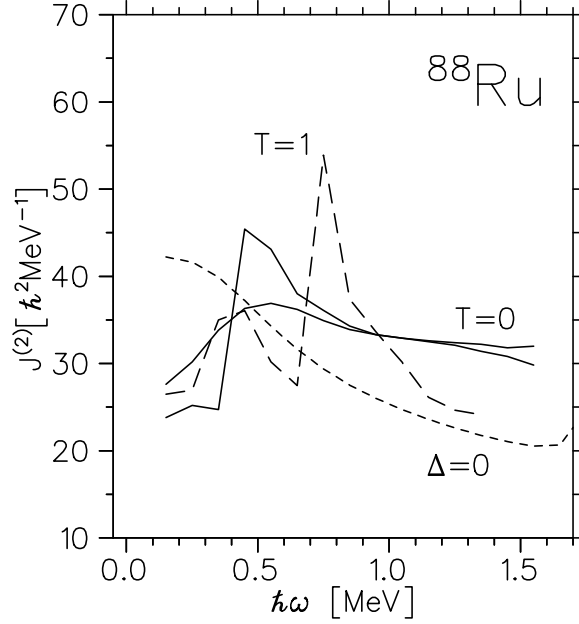
FIGURE 5. The J^2 moment of inertia resulting from the minimum of the TRS-calculations with different parameters of the pairing correlations. For further information, see text.

super-deformed nuclei, the fingerprints of $T = 0$ type pairing may become enhanced, especially at high angular momenta.

Results of our total routhian surface calculations are shown in Fig.5. We compare four different sets of calculations: The standard solution where we allow for $T = 1$ pairing only (dashed line), shows a sharp crossing related to the alignment of $h_{11/2}$ protons and neutrons. After that bandcrossing, the moment of inertia drops and approaches the curve, where no pairing correlations are present ($\Delta = 0$, short-dashed line). The curves shown with solid lines correspond to a calculation, where we allow both $T = 0$ and $T = 1$ pairing to be present. The strength of the $T = 0$ pairing field is scaled with respect to $T = 1$, see the discussion in [4]. The curve that shows only a smooth hump in the frequency range of $\hbar\omega \approx 0.5$ MeV has a strenght of $G_{T=0} = 1.3 G_{T=1}$, implying that the $T = 0$ pairing field is present already at $\hbar\omega = 0.0$ MeV. No sharp band crossing is observed for that case. When we choose a strength that is undercritical, $G_{T=0} = 1.1 G_{T=1}$, implying that the pairing is of $T = 1$ type at $\hbar\omega = 0.0$ MeV, we experience a pairing phase transition from $T = 1$ to $T = 0$, which is related to the sharp crossing at $\hbar\omega = 0.5$ MeV. This kind of transition has been discussed previously in Ref. [29]. and reflects the mean-field approximation.

Note that the moment of inertia for a rotational band, where $T = 0$ pairing correlations are present, exceeds by a far amount the value that is obtained for 'rigid' rotation (i.e. no pairing correlations). The nucleus appears thus more 'rigid' in the presence of $T = 0$ correlations. This is exactly the same phenomenon as discussed above concerning the band-termination. Since the angular momentum in a nuclues is built up from the contribution of individual nucleons, the angular momentum space is limited for each specific configuration. This is in contrast to a rigid body, where there is in principal no limitation, beyond fission. In the presence of $T = 0$ pairing, the configuration space is not limited anymore, since now the short range correlations will always scatter pairs into orbitals with larger angular momenta, and hence allow for an increase in angular momentum. Hence, rotation in that case really resembles the rotation of a rigid body, and the drop in the moment of inertia, which is obtained in all nuclei at a certain frequency, may not be observed.

CONCLUSIONS.

We have presented different model studies that explore the iso-spin degree of freedom in the particle-particle channel. The $T = 0$ pairing correlations are expeted to influence the structure of $N = Z$ nuclei. In order to discuss these correlations, one certainly cannot restrict to the narrow definition of $L = 0$ pairing. As shown for the case of a single j-shell, all L-values contribute to the correlations. In the context of the mean-field, it is clear that a $T = 0$

pairing gap is obtained, i.e. the correlations are coherent. The $T = 0$ pairing is resistant to rotation and modifies the rotational spectrum at high angular velocities. A new kind of collective excitation mode appears, allowing for smooth and continous occupation of high-j orbits.

ACKNOWLEDGEMENTS.

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